

# Models for Estimation of Chemical Distribution and Fate in Response to Remedial Alternatives in the Lower Willamette River

## Modeling Discussions Portland Harbor Superfund Project

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# Purpose

- \* Evaluate impact of source control activities and remedial action alternatives on chemical levels in:
  - Sediment, water column
  - Fish tissue
- \* Provide estimates of:
  - Loads from “unknown” external sources
  - Ambient levels in relation to PRGs
  - Probability of site recontamination
  - Contributions from outside the site (e.g., upstream)
  - Effects of monitored natural recovery
  - Downstream responses to actions upstream

# Response to remedial actions

## \* How much?

- Contributions from multiple sources
- Source reductions may not translate into a proportional reduction in sediment, water, fish

## \* How fast?

- Time constants of system components vary
- Temporal response of system will depend on which source is targeted for remediation

# Response to remedial actions

## \* How permanent?

- Sources are direct and indirect
- If ultimate source is not remediated, potential for recontamination will remain

## \* How extensive (spatially)?

- Local sediment vs. impacts from upstream sediment
- Downstream extent of response depends on both biological and physical processes

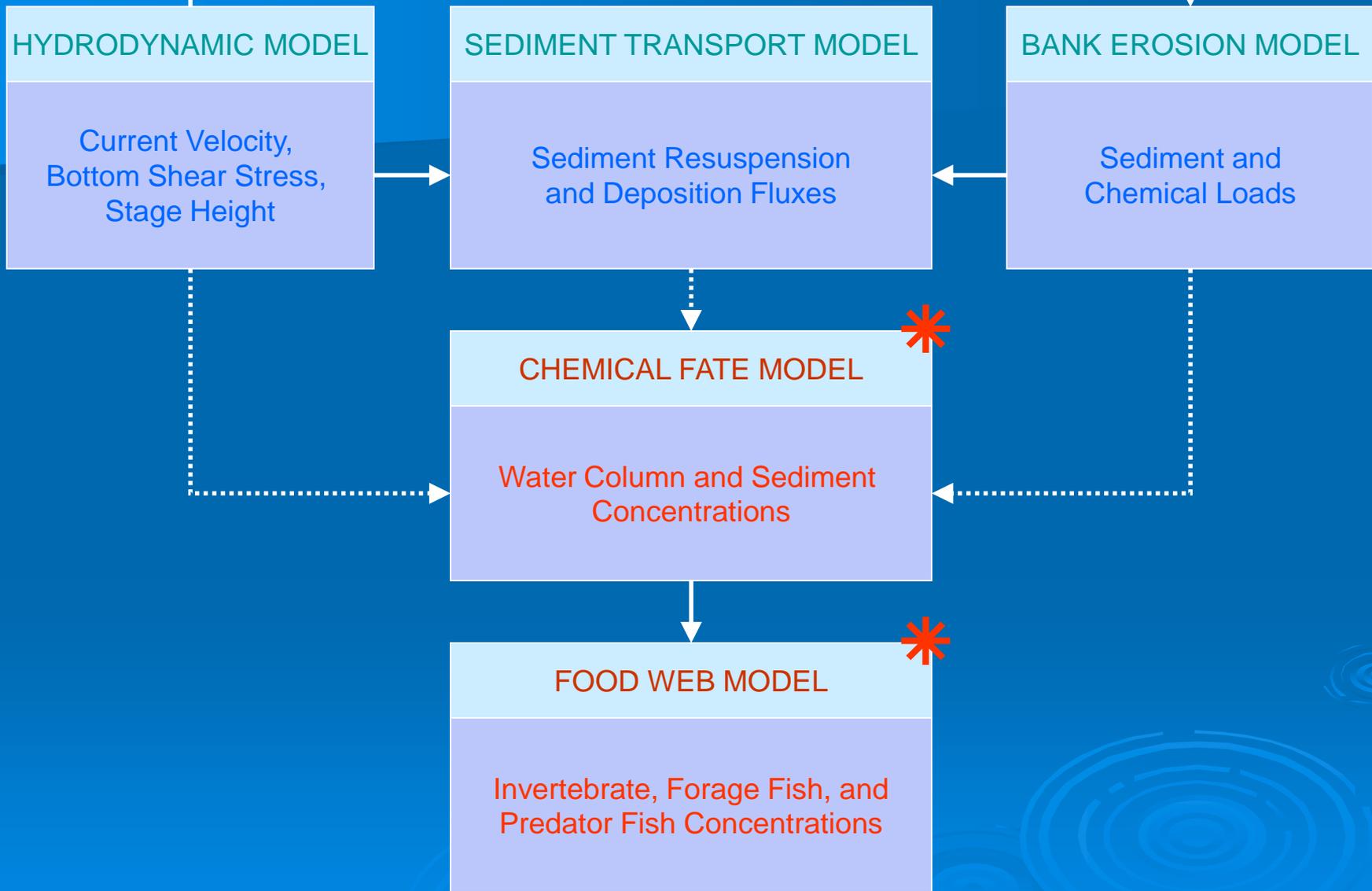
## \* How necessary?

- Actions may increase recovery rate
- Assessing “natural” attenuation in basis for remedial action

# A decision support tool

- \* A computer model, in conjunction with data analyses, may be used to quantitatively and comparatively address these primary study questions
- \* Use of a model may decrease uncertainty in effectiveness of the preferred remedy
- \* Benefits
  - Constrain, synthesize and interpret data
  - Compare remedial alternatives on same basis
- \* Drawbacks
  - Level of uncertainty in results may be unacceptable

Current Velocity



# Key specifications

## \* TRANSPARENCY

- \* Link transport & fate  $\Rightarrow$  food web models
- \* Incorporate spatial variability
  - Exposure of mobile species
- \* Incorporate temporal variability
  - Seasonal variation; Non-steady-state dynamics
- \* Evaluate organics and other chemicals
- \* Results as mass or concentration
- \* Food web-specific:
  - Invertebrates as whole animals, intra- and up-trophic consumption, model fish  $\Rightarrow$  bird  $\Rightarrow$  egg

# Development basis

- \* Linked biotic and abiotic sub-models
  - After Gobas et al. (1998) - Fraser River
- \* Abiotic - transport & fate sub-model
  - After Davis (2003, 2004) for San Francisco Bay
  - Considers back- and cross-flows between segments
  - STELLA®
- \* Biotic - food web sub-model
  - After Arnot & Gobas (2004)
  - Same generic structure in every segment
    - Multi-segment exposure for mobile species
    - Excel® & Visual Basic®

# Steps forward

## \* STEP 1

- Compile, analyze and synthesize available data
- Refine CSM
- Initial model development
- Decision point
  - Sufficient data for model calibration and validation?

## \* STEP 2

- Calibrate / corroborate sub-models
- Conduct sensitivity and uncertainty analyses
- Decision point
  - Model sufficiently constrained for a management tool?

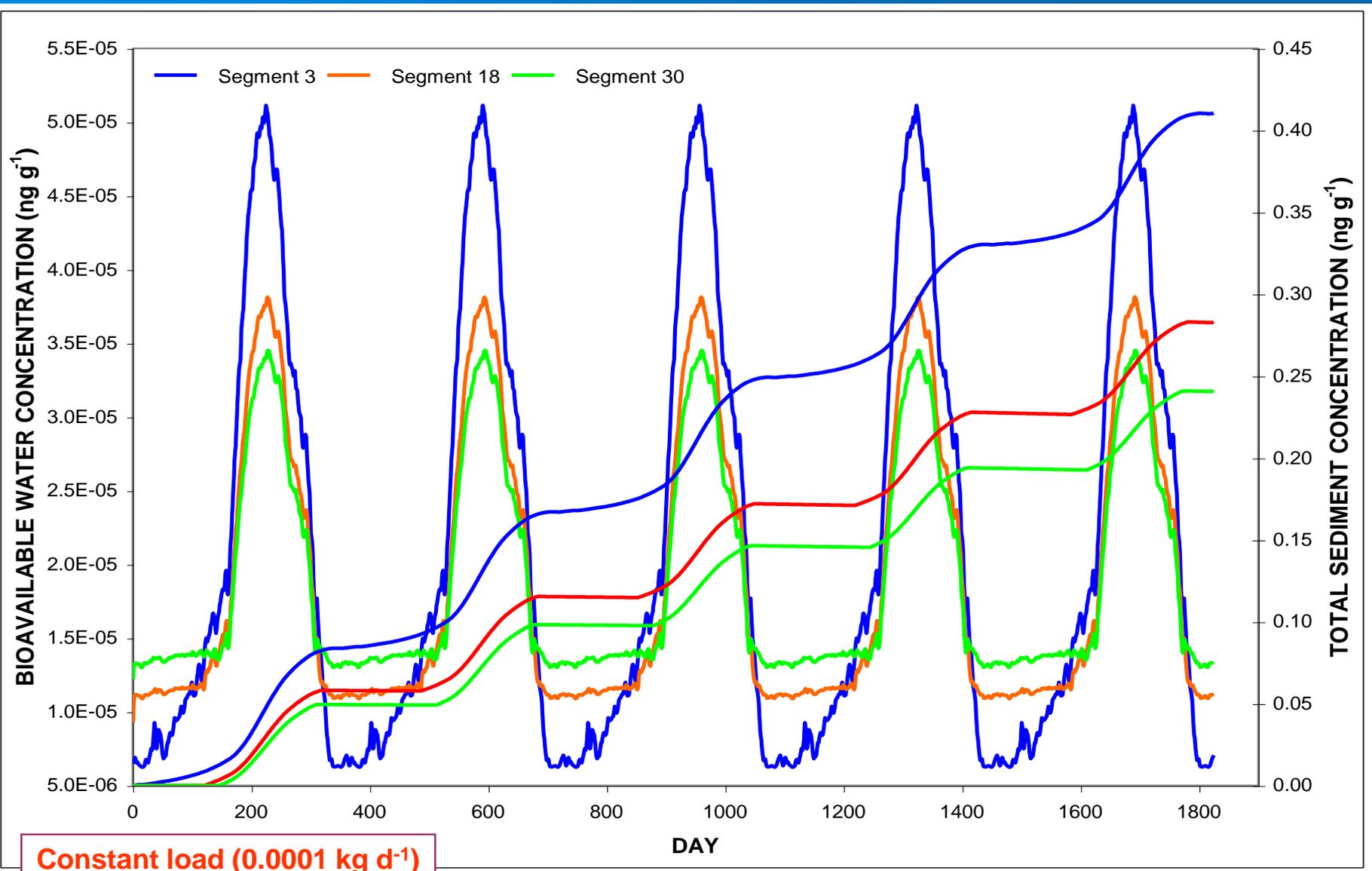
## \* STEP 3

- Conduct source analyses
- Evaluate impacts of various remedial alternatives

# EXAMPLE OUTPUT

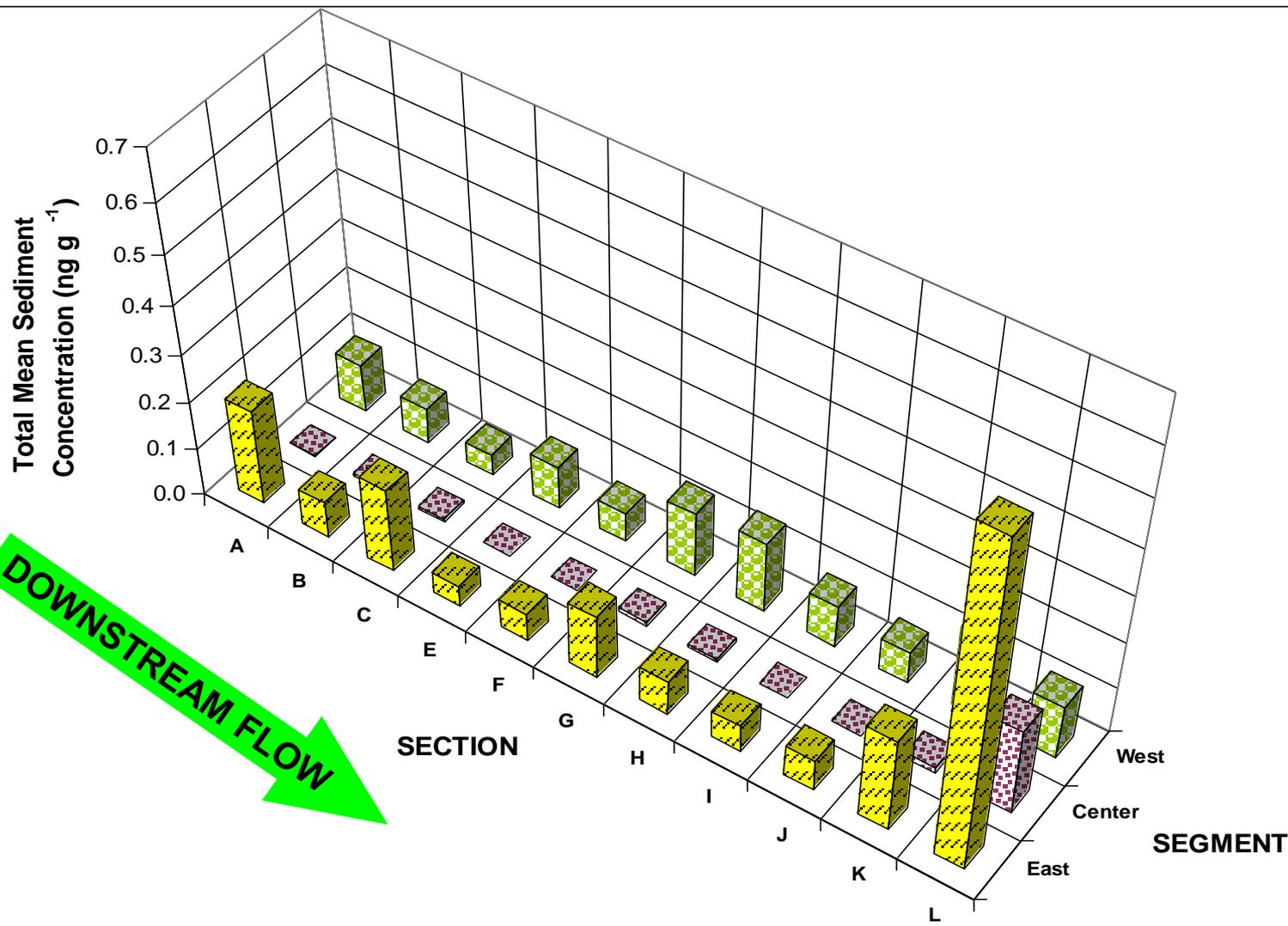


# Changes in water & sediment concentrations



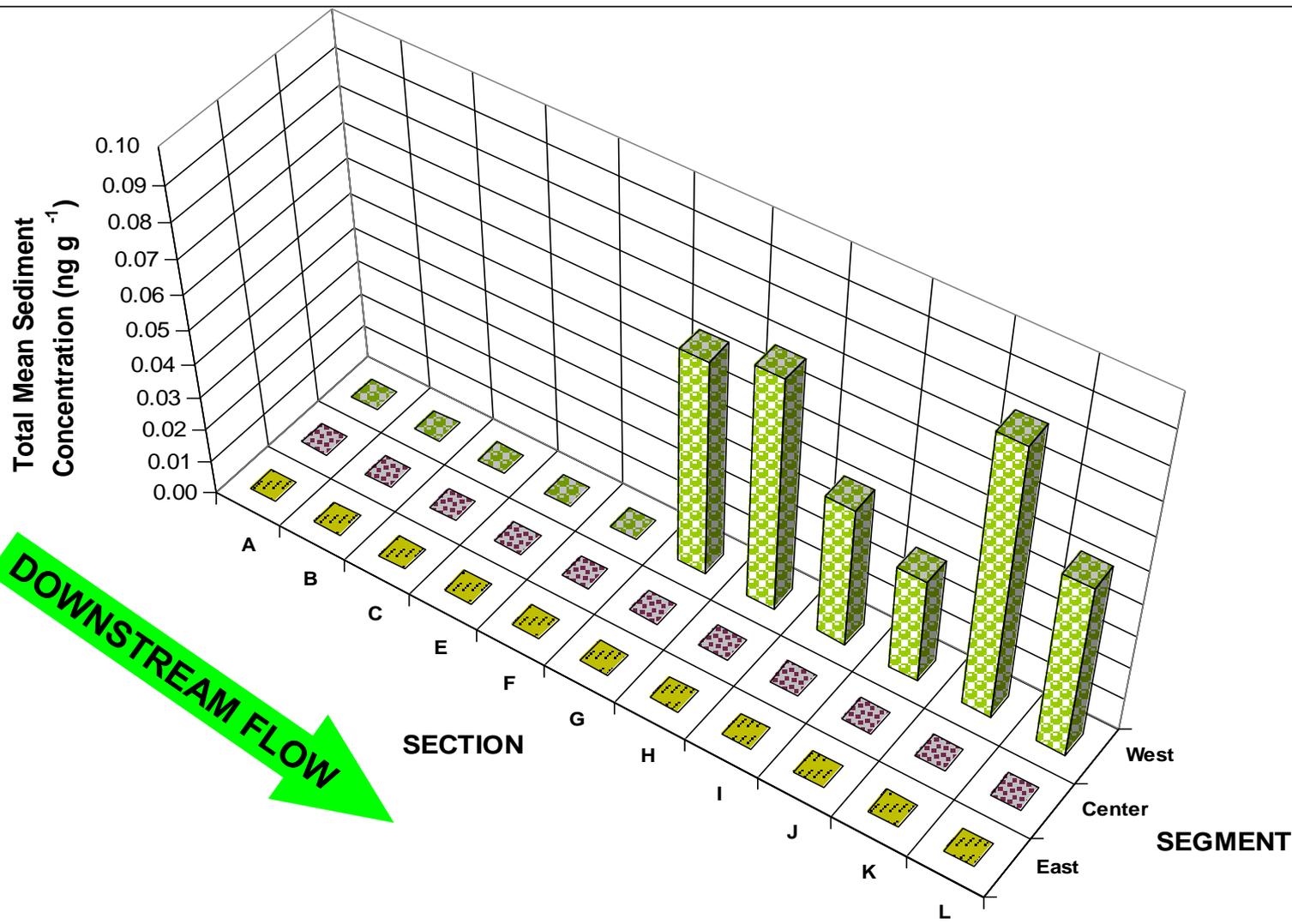
Constant load (0.0001 kg d<sup>-1</sup>)  
to water in segments 1,2,3

# Changes in sediment concentration across segments



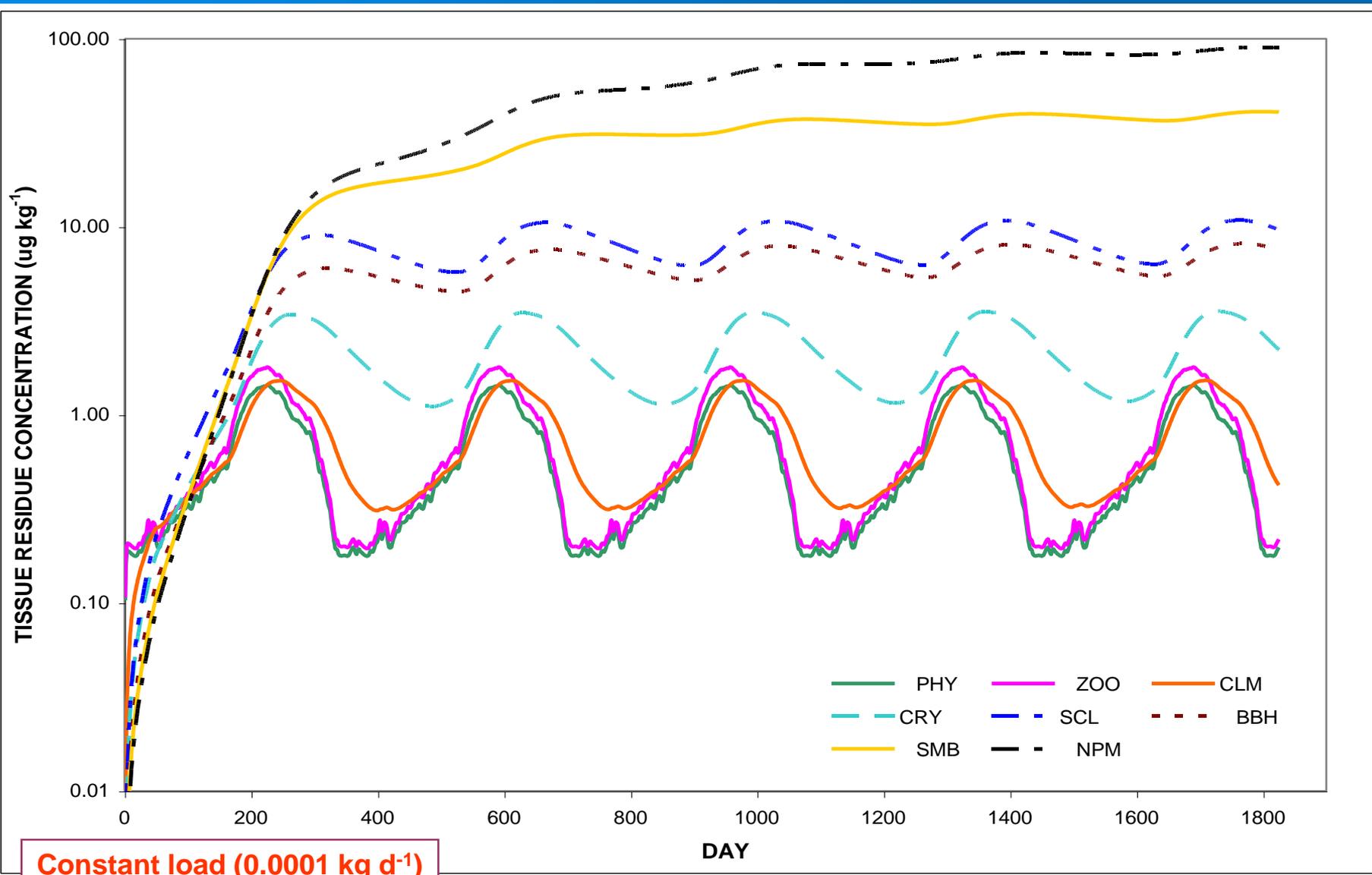
Constant load ( $0.0001 \text{ kg d}^{-1}$ )  
to water in segments 1,2,3

# Changes in sediment concentration across segments



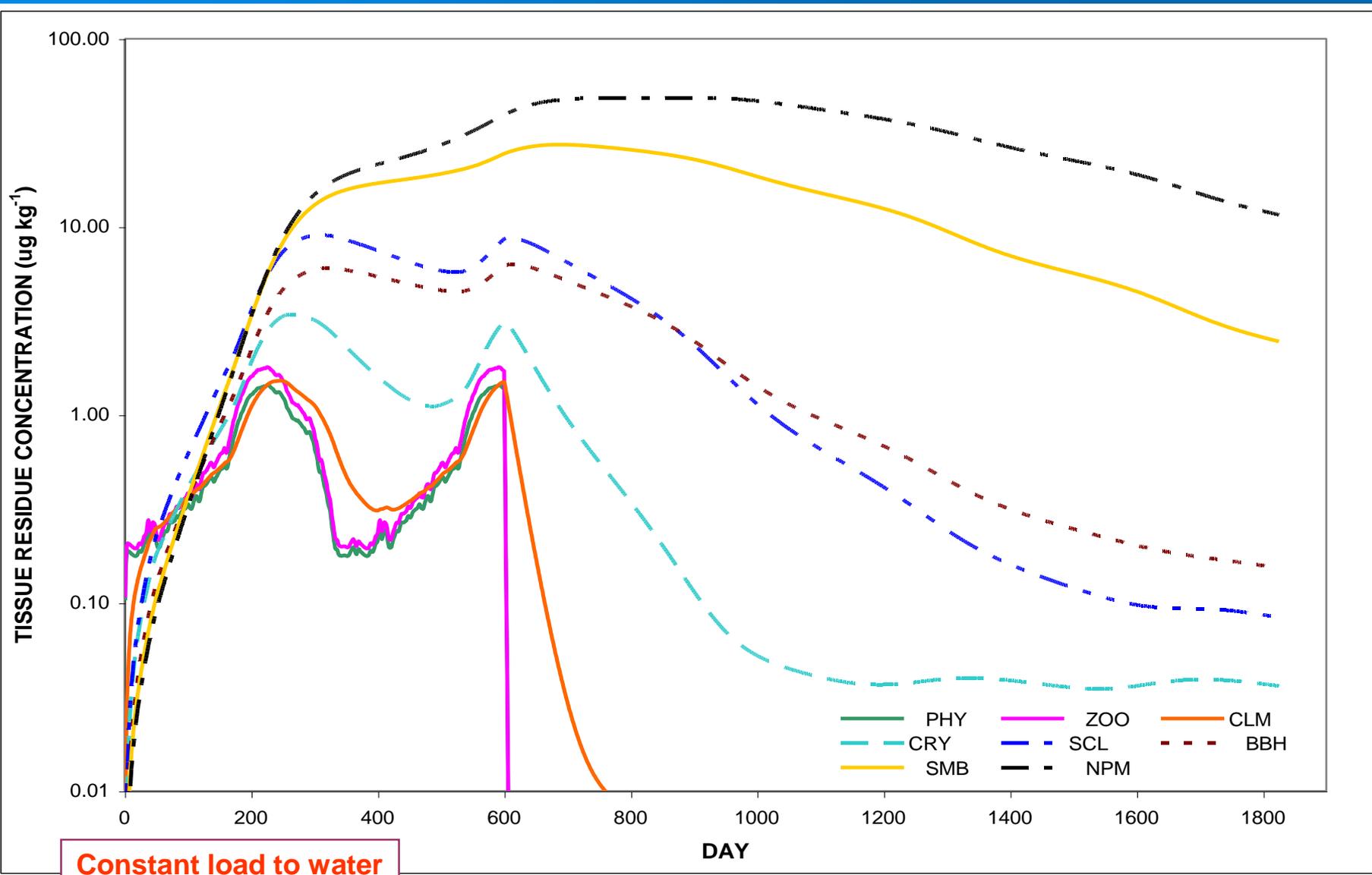
Constant load (0.0001 kg d<sup>-1</sup>)  
to water in segment 16

# PCB-118 tissue residues over time (baseline)



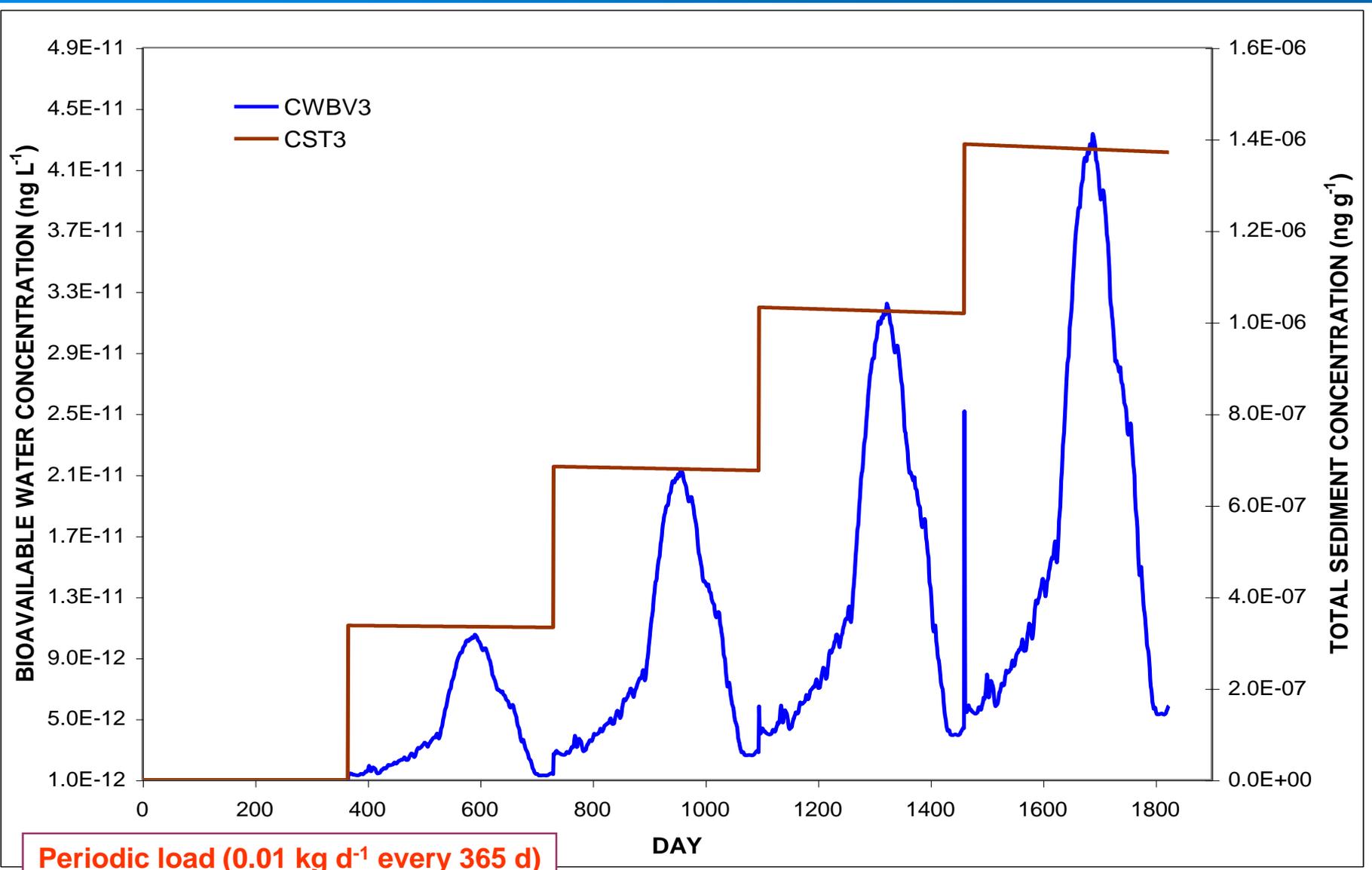
Constant load ( $0.0001 \text{ kg d}^{-1}$ )  
to water in segments 1,2,3

# PCB-118 tissue residues over time (post-remedy)



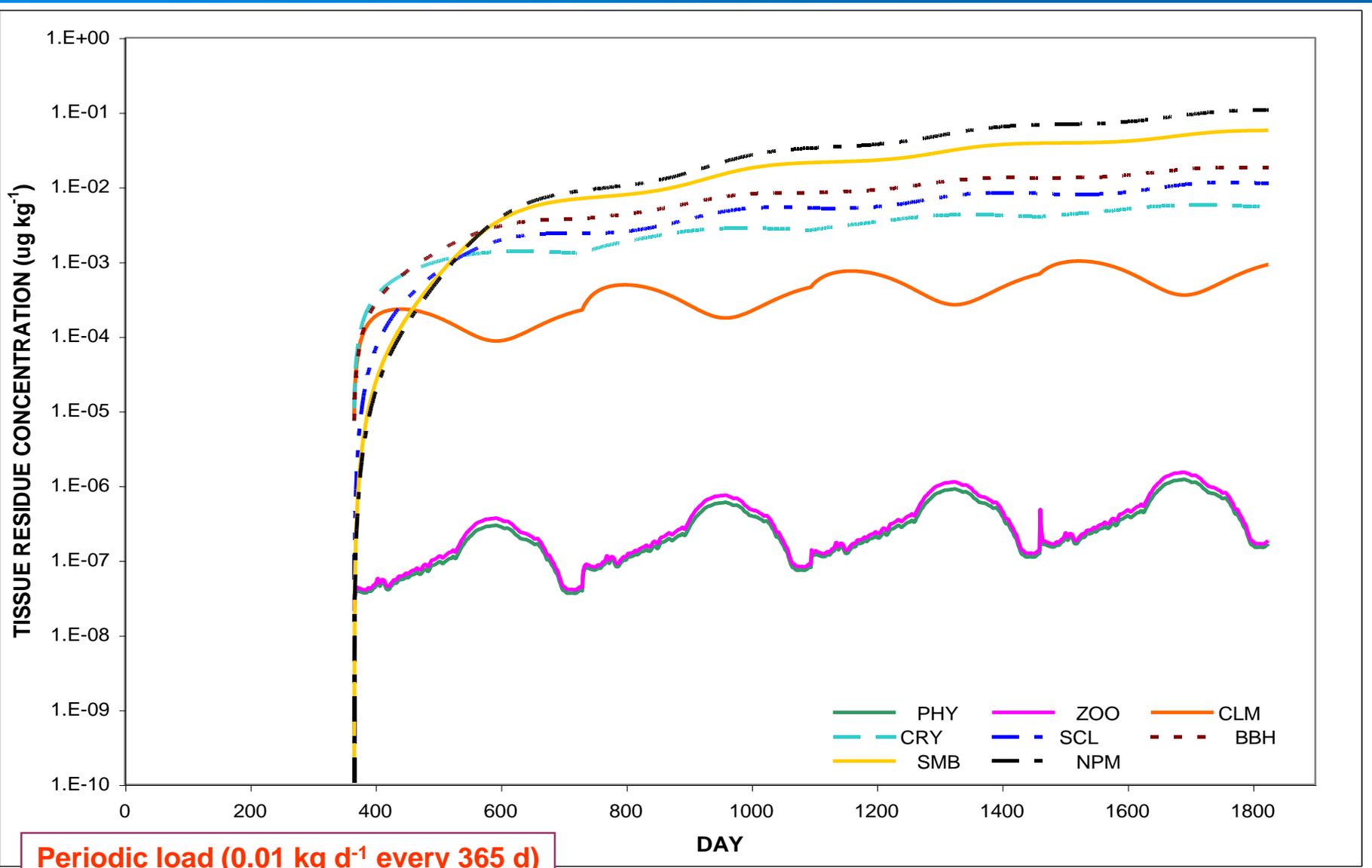
Constant load to water ceases at t = 600 d

# Changes in water & sediment concentration (periodic)

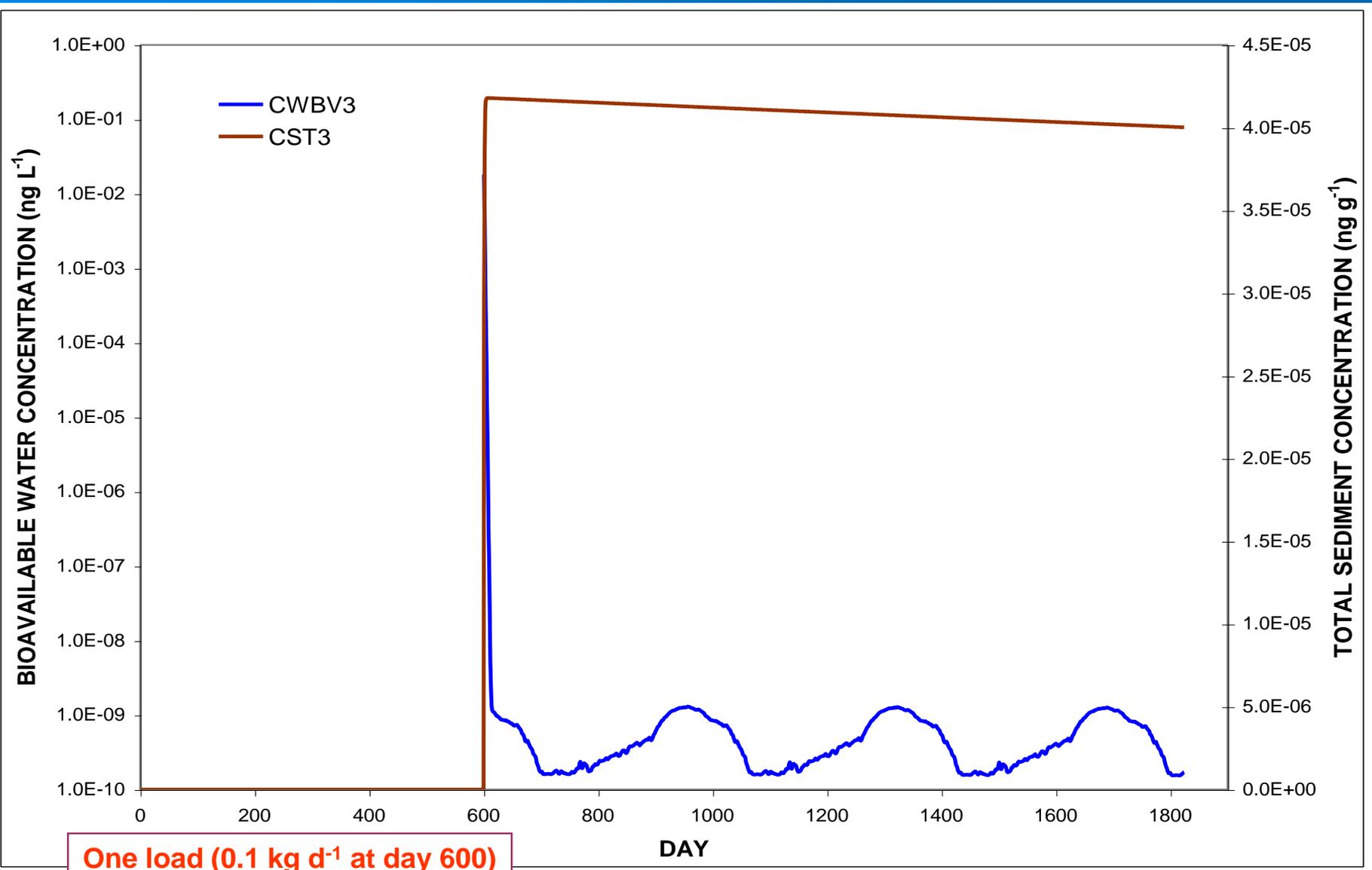


Periodic load (0.01 kg d<sup>-1</sup> every 365 d)  
to water in segments 1,2,3

# PCB-118 tissue residues over time (periodic)

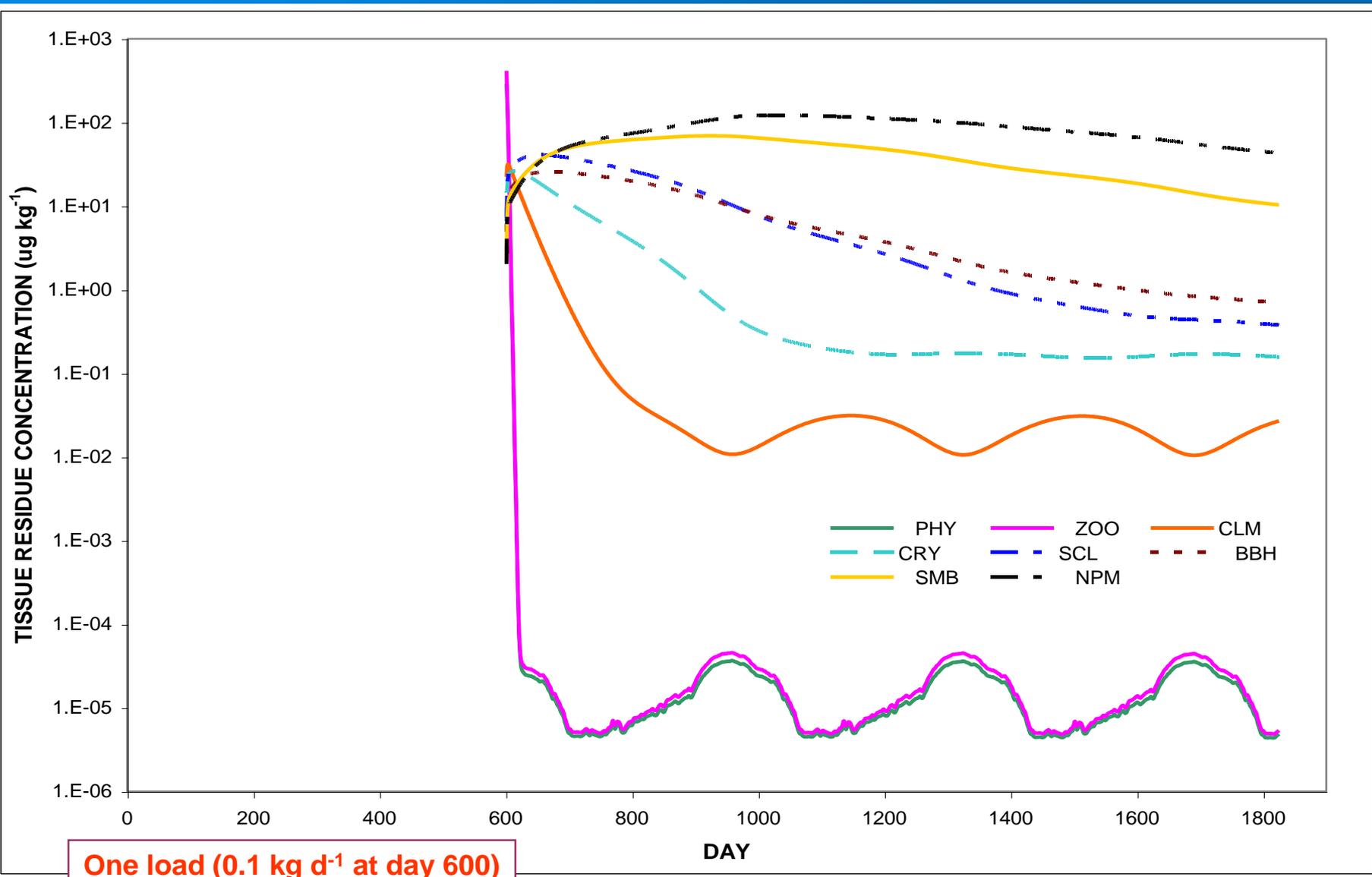


# Changes in water & sediment concentration (one load)



One load (0.1 kg d<sup>-1</sup> at day 600)  
to water in segments 1,2,3

# PCB-118 tissue residues over time (one load)



One load ( $0.1 \text{ kg d}^{-1}$  at day 600)  
to water in segments 1,2,3

# OVERVIEW OF MODELS



# Contaminants

## \* POLYCYCLIC AROMATIC HYDROCARBONS

- Naphthalene
- Phenanthrene
- Fluoranthrene
- Benz(a)anthracene
- Benzo(b)fluoranthene
- Dibenz(a,h)anthracene
- Benzo(ghi)perylene

## \* METALS

- Mercury (methylmercury)
- Arsenic
- Other

## \* POLYCHLORINATED BIPHENYLS

- PCB 18
- PCB 66
- **PCB 118**
- PCB 153
- PCB 194

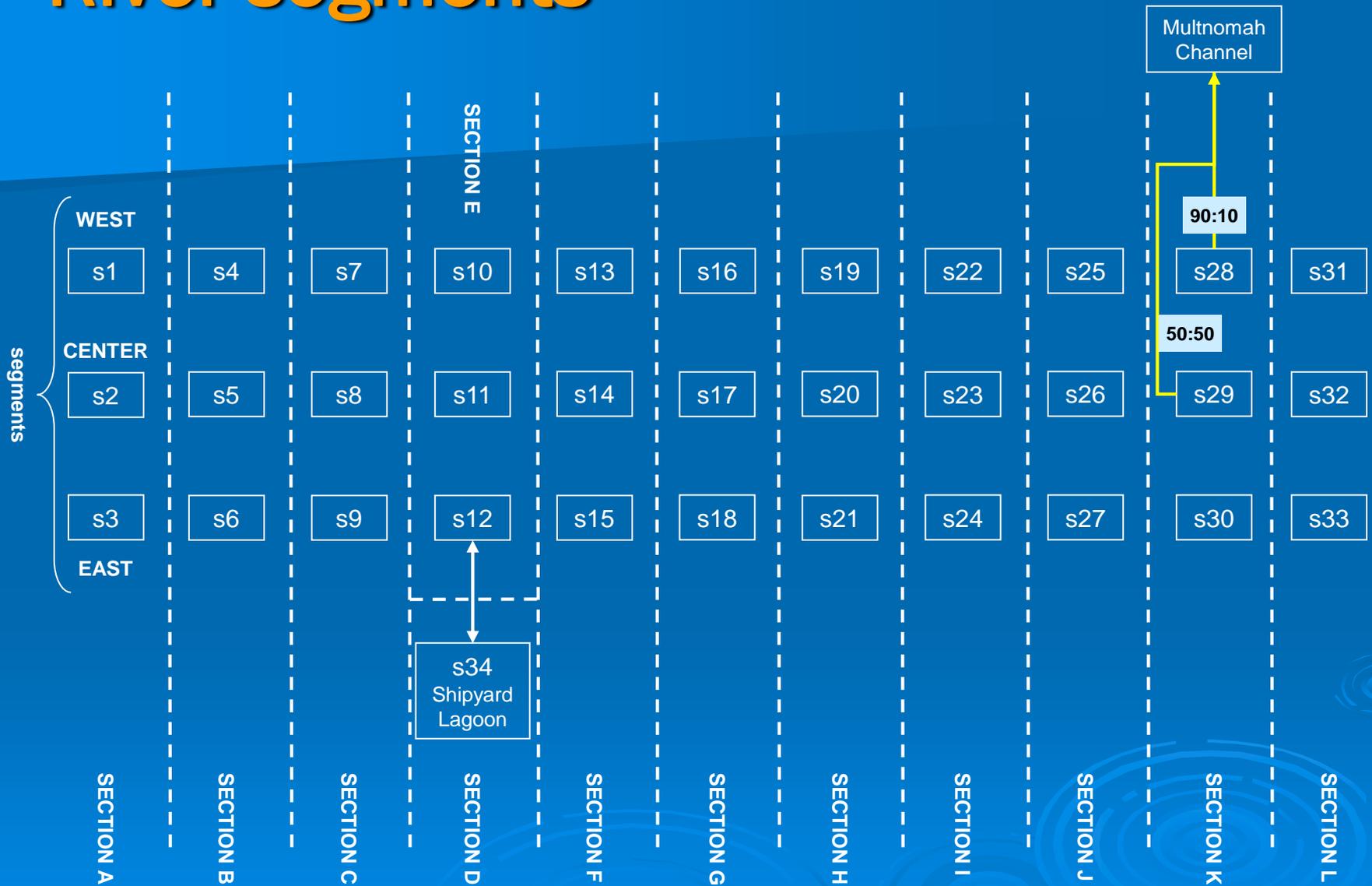
## \* DIOXINS

- TCDD, PCDD, HCDD

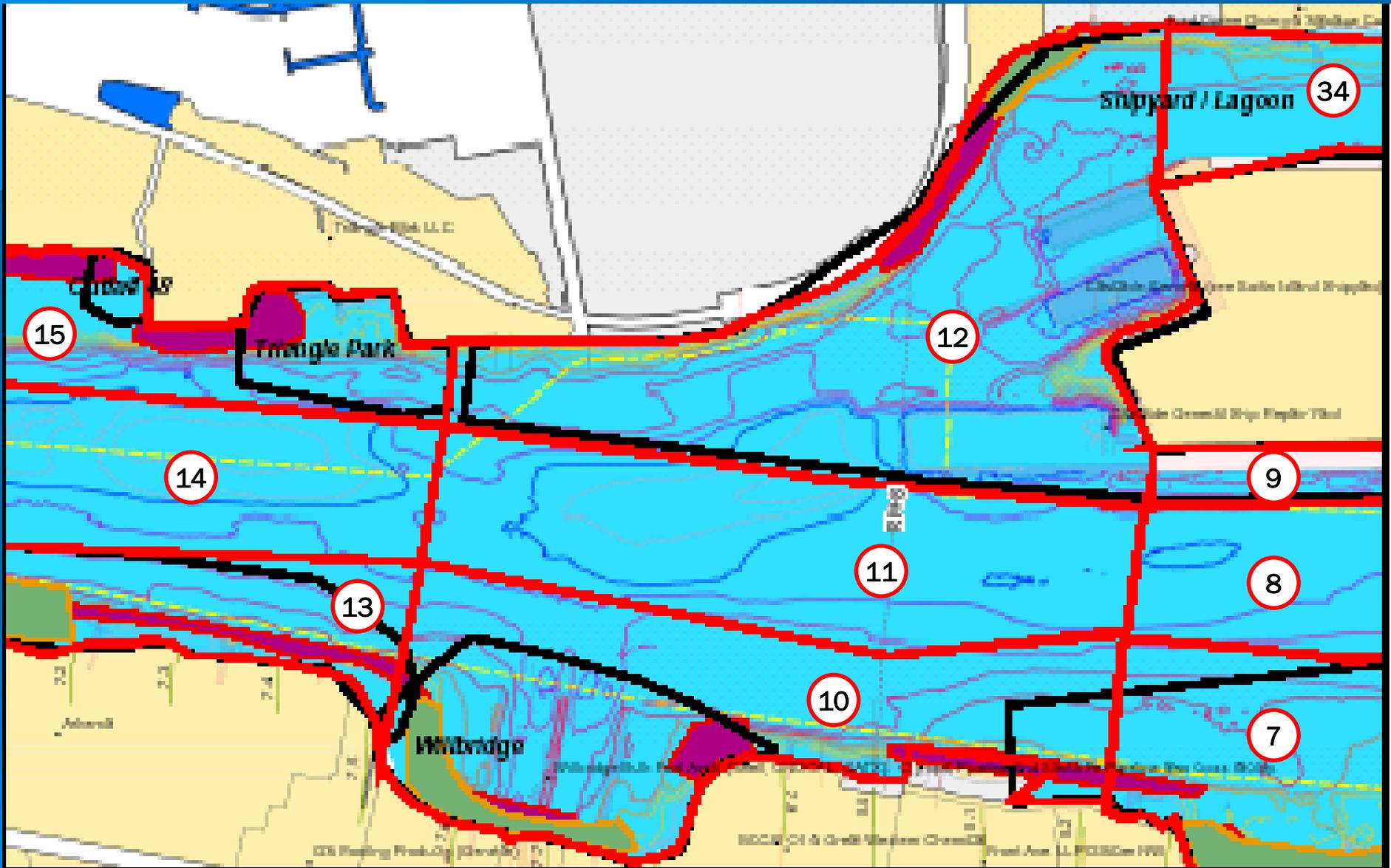
## \* PESTICIDES

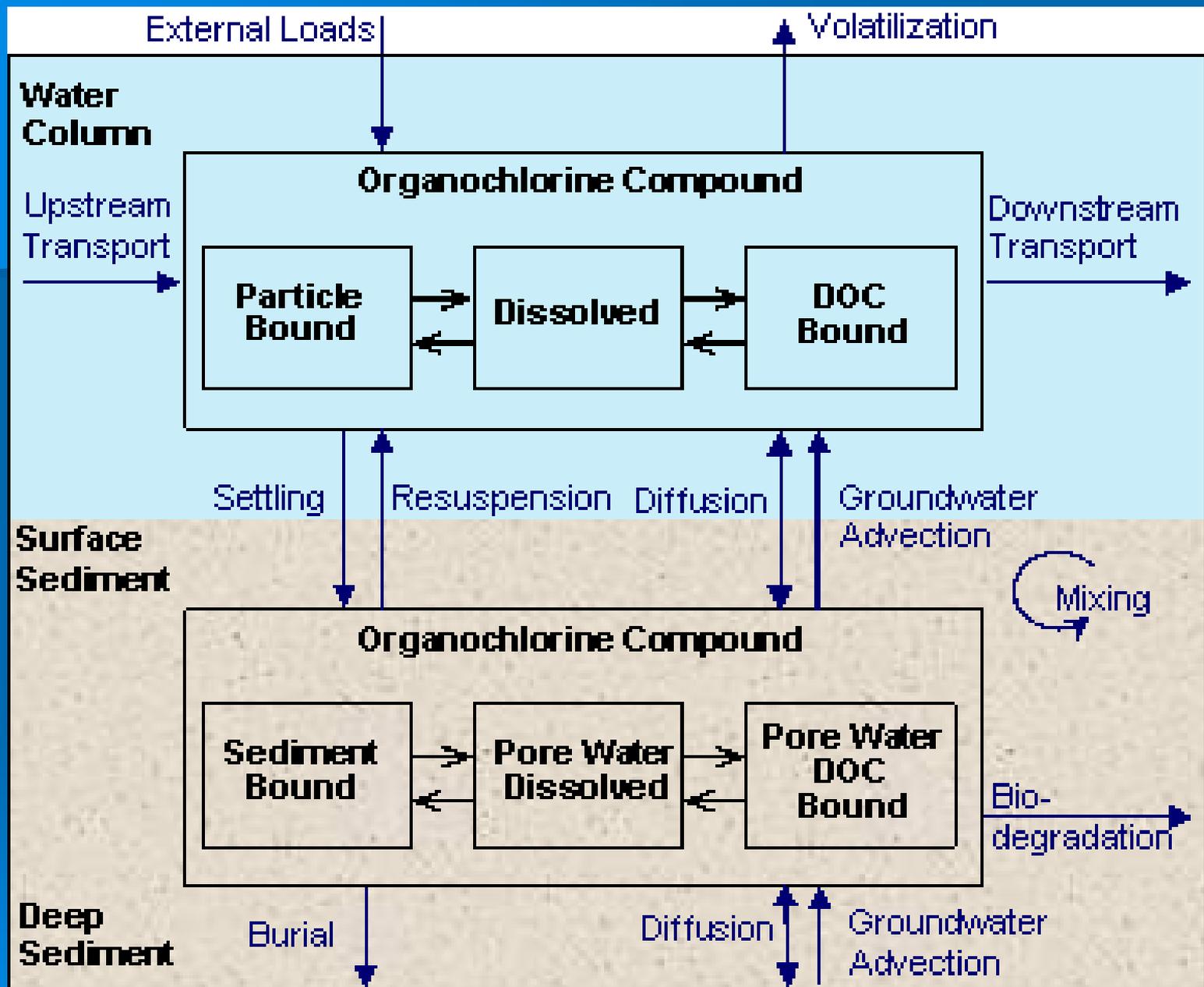
- DDT
- DDE
- DDD

# River segments

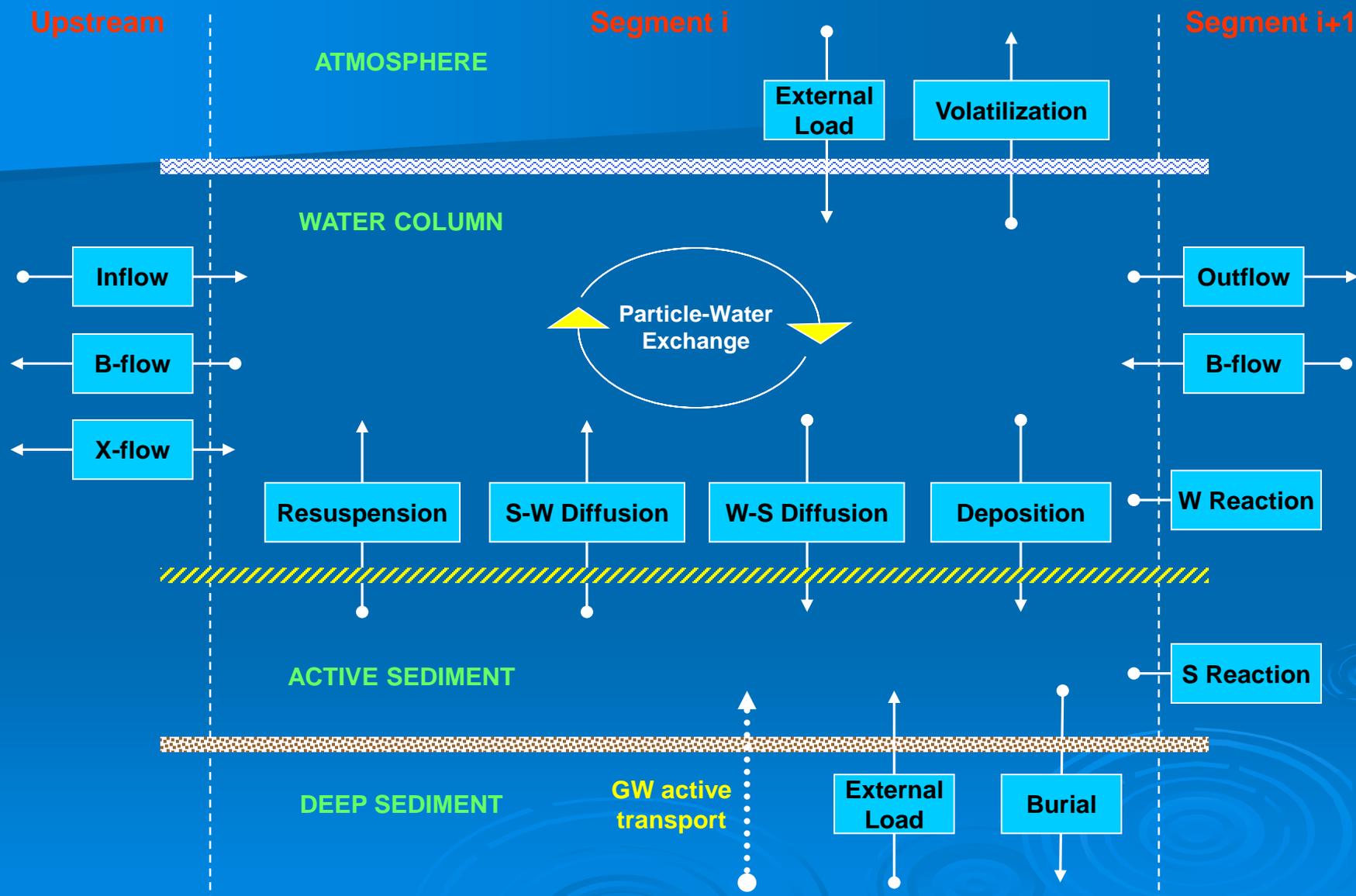


# Segments mapped to the physical river

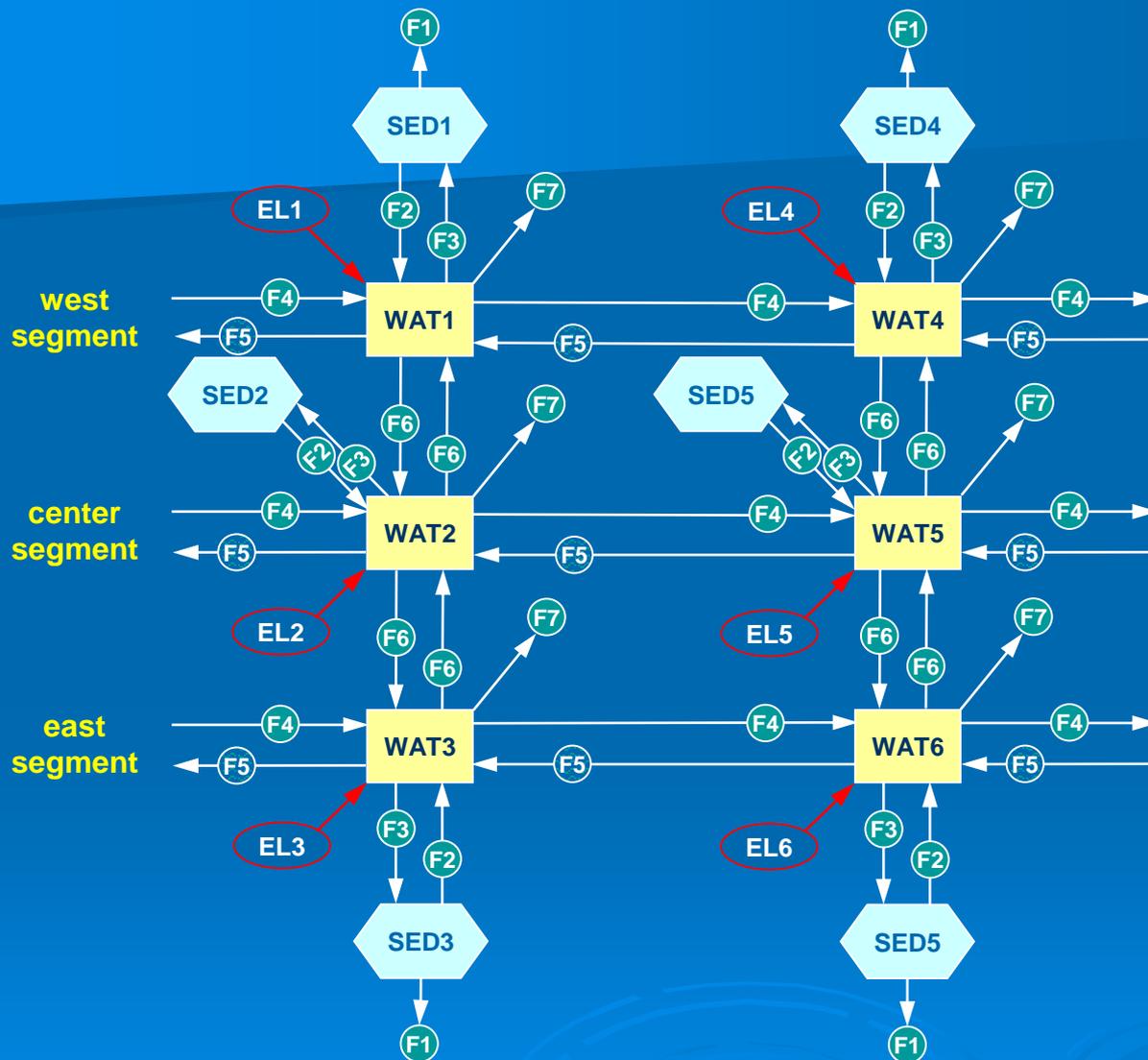




# Transport & fate sub-model for a single river segment

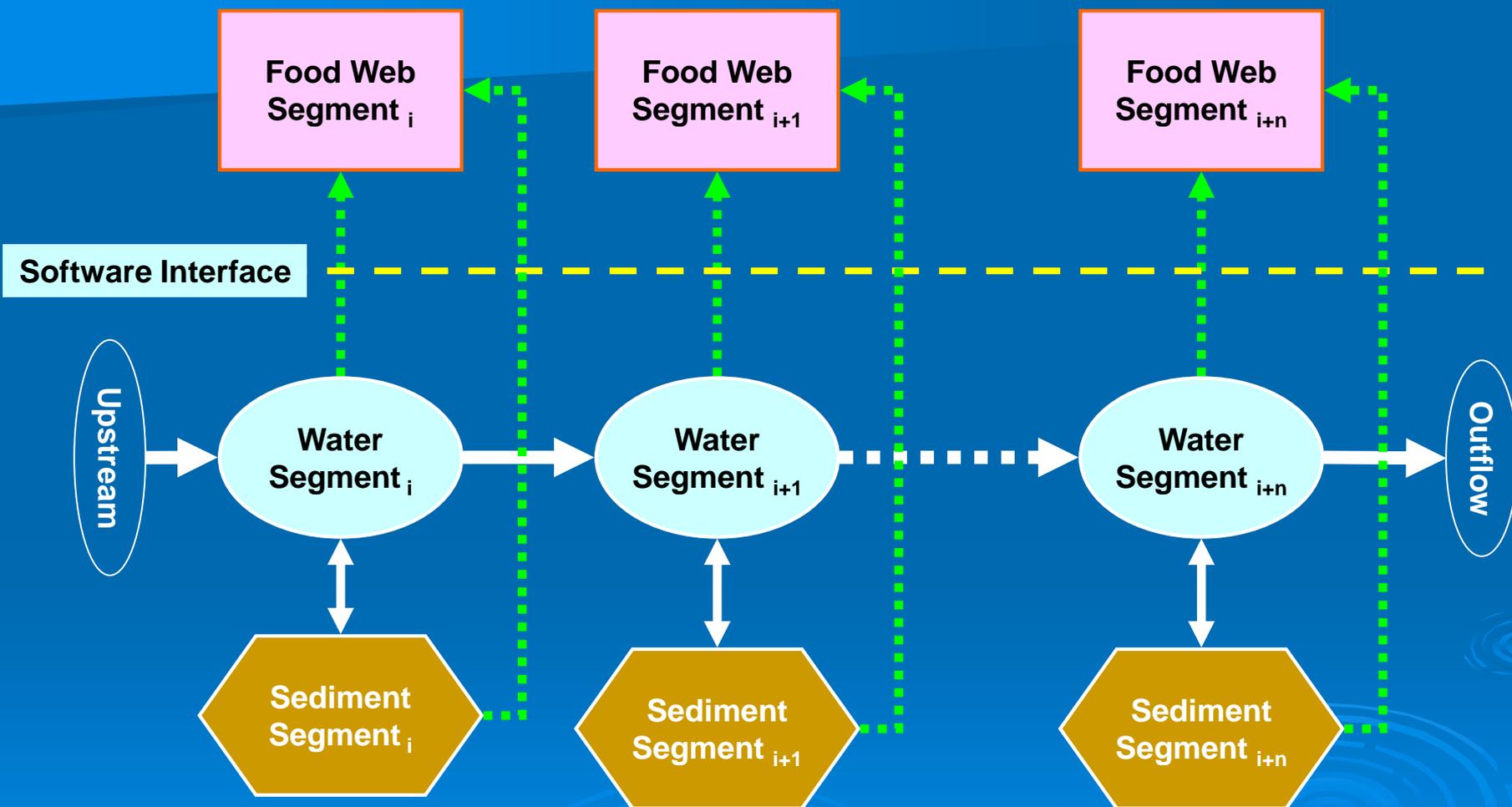


# Abiotic sub-model relationships between segments



# Sub-model linkages over multiple segments

## FOOD WEB (BIOTIC) SUB-MODEL

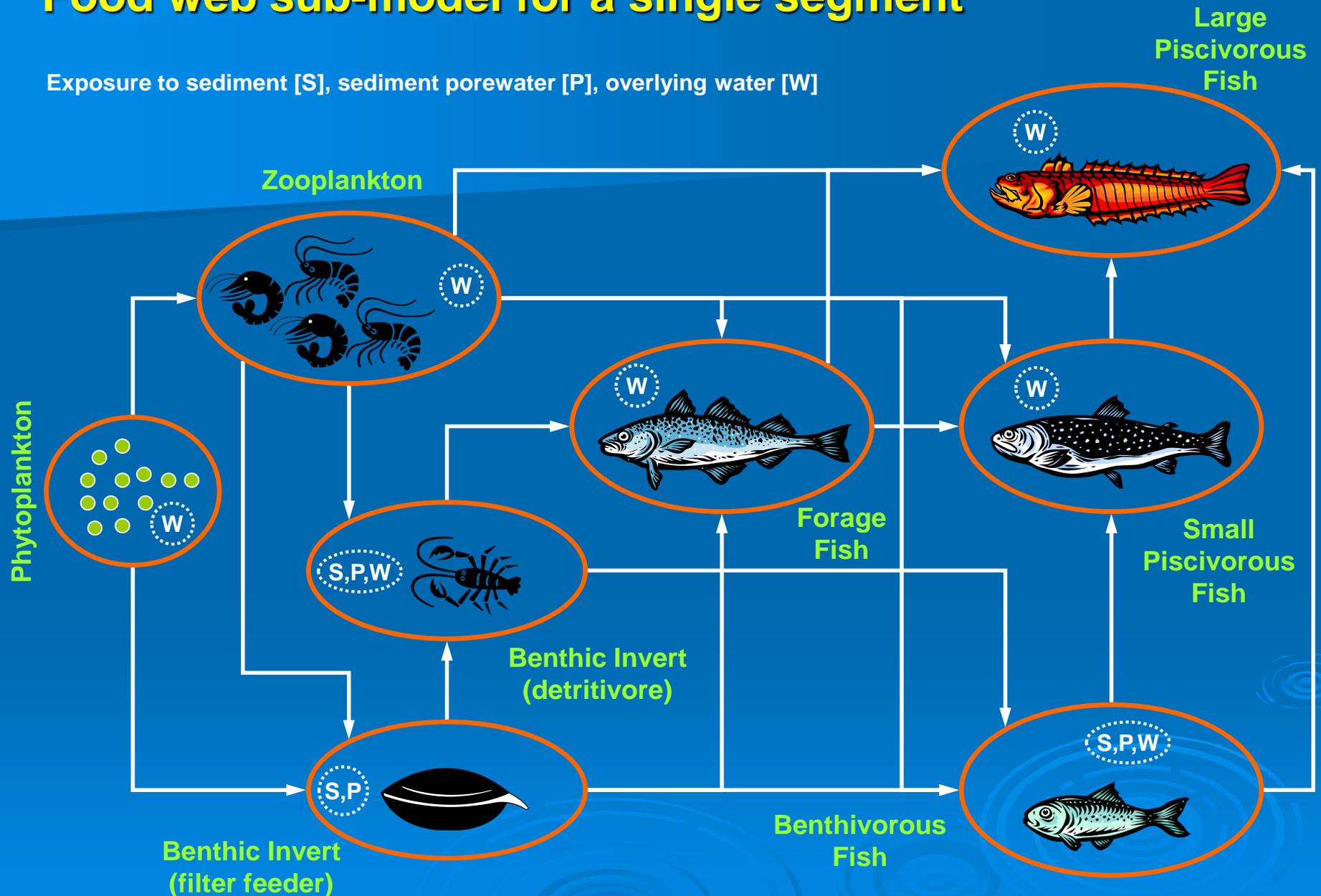


## TRANSPORT & FATE (ABIOTIC) SUB-MODEL

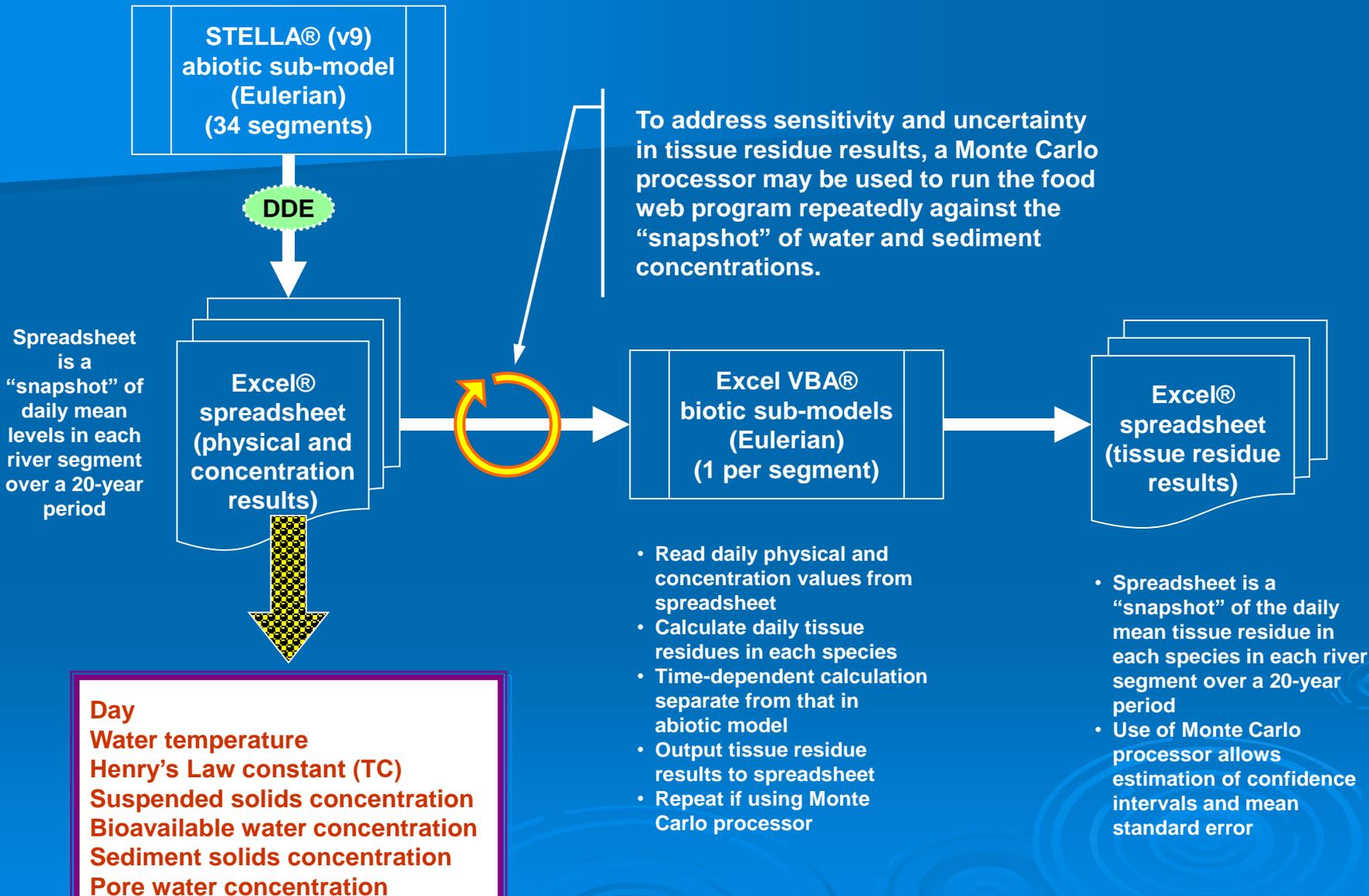
Portland Harbor Modeling Discussions (May 2006)

# Food web sub-model for a single segment

Exposure to sediment [S], sediment porewater [P], overlying water [W]



# Data flow and manipulation between sub-models



# Most sensitive parameters

- ~\* Henry's Law constant
- ~\* Octanol-water partition coefficient
  - \* Water temperature
- ~\* River flow rate
  - \* Active sediment depth
  - \* Concentration of solids in sediment
  - \* Density of particles (suspended) in water
  - \* Sediment solids burial rate
- ~\* Bioavailable concentration in water (+ related terms)
  - \* Water content fraction of organism (~ lipids)
  - \* Dietary fraction(s)